On kinetic energy stabilized superconductivity in cuprates

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The possibility of kinetic energy driven superconductivity in cuprates as was recently found in the tJ model is discussed. We argue that the violation of the virial theorem implied by this result is serious and means that the description of superconductivity within the tJ model is pathological.

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Recent numerical simulations and analytical studies of the Hubbard and tJ models, which suggest that superconductivity in doped cuprates may be driven by a lowering of kinetic energy upon formation of the superconducting state[1,2,3,4,5,6,7,8,9,10,11] have resulted in considerable interest, including spectroscopic measurements and their interpretation.[12,13,14] The essential physics depends on the replacement of the full Hamiltonian and electronic degrees of freedom by a limited number of degrees of freedom associated with the charges of the doped carriers within a stiff background related to the electronic structure of the undoped antiferromagnetic Mott insulating cuprate phases, which motivate these models. Within this antiferromagnetic background paired carriers can be more mobile than single carriers, and this can overcome the normal increase in kinetic energy upon pair formation. As was already mentioned, such an increase in kinetic energy is unusual as normally the virial theorem of Clausius would prevent it, but it has been argued that this is allowed within the tJ model, and that the kinetic energy as defined within the tJ model is a more physical quantity than the kinetic energy of the full electronic system.[1]

The purpose of this short paper is to argue that this apparent violation of the virial theorem is serious, and implies that if the result that superconductivity in the tJ model is kinetic energy driven is correct, then the tJ model is pathological in the sense that its superconductivity is essentially different from that in the cuprates, or that it neglects degrees of freedom that are essential for obtaining the superconducting state, or both.

To a very good approximation, solids, including cuprates, may be regarded as bound systems composed of nuclei and electrons interacting via the Coulomb potential. While highly precise, this view is generally useless without approximations and effective models that capture the physics of interest and the relevant degrees of freedom within a tractable framework. Constructing such models is crucial for progress, not only because they make calculations possible, but also because by reducing the number of degrees of freedom to a smaller number of approximate degrees of freedom that can be physically interpreted, they provide understanding of the essential physics. However, exact results and scalings, based on the bare system are useful in constraining effective models and defining their range of applicability. For example, the use of exact scalings for the electron gas has proved to be of considerable value in the construction of generalized gradient approximations for density functional studies of solids.[15,16]

According to the virial theorem for a stable bound system of interacting Coulomb particles,[17,18,19] the kinetic energy, T, which is positive, is equal to -1/2 of the potential energy, V, which is negative with standard definitions. Thus the energies of eigenstates are ordered such that lower energy corresponds to higher kinetic energy. This applies also to a variety of other local potentials and to relativistic systems. Since the superconducting state in cuprates is a ground state, or if not, it is at least a lower energy state than the ensemble that comprises the normal state at finite temperature (the specific heat is positive), the virial theorem implies that the conventional kinetic energy in the superconducting state is unambiguously higher than that in the normal state.

Therefore, in cuprates, using conventional definitions of potential and kinetic energy, superconductivity is driven by a reduction in potential energy, accompanied by a smaller increase in kinetic energy. Norman and co-workers[20] have discussed the relationship between the condensation energy and electronic spectral functions, especially as related to angle resolved photoemission. They emphasize that while the virial theorem applies to the full Hamiltonian, it need not apply in a reduced subspace, e.g. the space of low energy electronic excitations. In any case, a simple interpretation of the above would be that the tJ model describes an unphysical superconductivity. However, the situation may not be so simple. First of all, as was suggested already,[1] the kinetic energy may be redefined as the kinetic energy of the lower Hubbard band, and this is essentially the quantity that decreases in the tJ model. Secondly, it may be argued that the kinetic energy overall increases, but that the kinetic energy relevant for excitations up to some cut-off energy decreases. However, both of these scenarios, which are related, would require that there be a larger kinetic energy increase involving degrees of freedom not included in the tJ model. This means that the main physics driving superconductivity is not in the tJ model, or that the kinetic energy of the tJ model is to be interpreted as mainly potential energy of the bare Hamiltonian, which would be difficult to understand since it originates in the hopping term.

We now turn to the origin of the virial theorem violation in the tJ model and speculate about possible ways

forward. As mentioned, the kinetic energy decrease into the superconducting state of the tJ model is apparently connected with the stiff antiferromagnetic Mott insulating background into which a small number of carriers are doped in this view of cuprate superconductivity. However, while the phase diagrams of cuprate superconductors generally show prominent Mott insulating phases at zero doping, these are separated from the superconducting phases. The superconducting transition is between a high temperature conducting state, with specific heat and other thermodynamic properties similar to a high carrier density metal and a unconventional superconductor. In general, the Fermi surfaces in the normal state, as measured by a variety of probes, are consistent with a high carrier density.[21] The transport, on the other hand, especially in the underdoped regime, shows a variety of non-Fermi liquid scalings, for example, linear in T resistivity. The non-Fermi liquid scalings evolve continuously into conventional metallic behavior with increasing hole doping above the optimum for T_c. These unconventional scalings can be reproduced within the framework of strong correlated models, based on doping of an underlying Mott insulating state.[11] However, it should be noted that the Mott insulator – metal transition is thought to be first order in clean cuprates, and therefore the connections between the Mott insulating phase and the conducting phase need not be taken for granted. Non-Fermi liquid scalings occur in other correlated materials that cannot be regarded as doped Mott insulators, for example, metals near quantum critical points.[22,23]

The importance of retaining charge degrees of freedom, not included in the tJ model has also been discussed as by Phillips and co-workers[24,25] both from the point of view of assymptotic freedom and from the metallic character.

The spin-charge separation that occurs in the tJ model and is expected in lightly doped Mott insulators, is not essential for non-Fermi liquid scalings in transport nor is the stiff antiferromagnetic background. Soft fluctuations that scatter charge carriers would suffice. In fact, based on neutron scattering experiments[26,27,28] and analysis of nuclear magnetic resonance (NMR) data,[29] the antiferromagnetic correlation length strongly decreases with doping and is $\sim$ 3 lattice spacings or less at optimal doping. This may be important both for the normal state properties and the superconductivity, although we note that a theory for cuprate superconductivity has not yet been established. A scenario in which doped cuprates are high carrier density metals with strong T-dependent scattering due to a nearby quantum critical point is more likely if the soft quantum fluctuations have a short coherence length, than if they are due to a sharply peaked (in Q) structure. This is because in the former case there is a larger phase space for fluctuations, and therefore a stronger quantum suppression of the underlying instability and more scattering. This can be seen from the fluctuation dissipation theorem, which relates the imaginary part of the susceptibility and the fluctuation amplitude.[30,31,32,33] Furthermore, within a spin-fluctuation pairing Migdal-Eliashberg framework, fluctuations with a short coherence length such that the inverse coherence length is of the order of the reciprocal space length scale for variation of the $d_{x^2-y^2}$ order parameter on the Fermi surface (i.e. $\sim$ 3-4 lattice spacings), would be more effective for pairing than sharply peaked fluctuations at the antiferromagnetic wavevector.[29,33] This is again because of phase space arguments, specifically that increasing the coupling at a specific k leads to ordered antiferromagnetism, while increasing the range of k involved strengthens the overall pairing without producing a magnetic instability.

In any case, assuming that calculations showing kinetic energy driven superconductivity in the tJ model for cuprates are correct, we argue that the tJ model is insufficient for understanding superconductivity in cuprates. One avenue for going forward may be to add more degrees of freedom in extended models to produce a softer, more metallic normal state especially in the charge channel. By removing the stiff nearly antiferromagnetic Mott insulating background, this may destroy the artificial kinetic energy driven tJ model superconductor in favor of a superconducting state consistent with the virial theorem.

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